Sensitivity of process design to uncertainties in property estimates applied to extractive distillation

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Sensitivity of process design to uncertainties in property estimates applied to extractive distillation

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Abstract

During the design of a chemical process engineers typically switch from simple (shortcut) calculations to more detailed rigorous models to perform mass and energy balances around unit operations and to design process equipment involved in that process. The choice of the most appropriate thermodynamic and thermo-physical models is critical to obtain a feasible and operable process design and many guidelines pertaining to this can be found in the literature. But even if appropriate models have been chosen, the user needs to keep in mind that these models contain uncertainties which may propagate through the calculation steps to such an extent that the final design might not be feasible or lead to poor performance. Therefore it is necessary to evaluate the sensitivity of process design to the uncertainties in property estimates obtained from thermo-physical property models. Uncertainty and sensitivity analysis can be combined to determine which properties are of critical importance from process design point of view and to establish an acceptable level of accuracy for different thermo-physical property methods employed. This helps the user to determine if additional property measurements in the laboratory are required or to find more accurate values in the literature. A tailor-made and more efficient experimentation schedule is the result. This work discusses a systematic methodology for performing analysis of sensitivity of process design to uncertainties in property estimates. The application of the methodology is illustrated using a case study of extractive distillation in which acetone is separated from methanol using water as a solvent. Among others, the vapour pressure of acetone and water was found to be the most critical and even small uncertainties from -0.25 % to +0.75 % in vapour pressure data have shown a significant impact on the reflux ratio of the extractive distillation process.
In general, systematic sensitivity analysis should be part of process design efforts and expected to contribute to better-informed and reliable design solutions in chemical industries.

1. Introduction

Property prediction models are used to describe the behaviour of chemical systems. Engineers shift from ideal state models for performing less precise calculations to more rigorous descriptions of a chemical system's behaviour. These rigorous models use parameters which have been estimated by regressing the experimental data of a wide range of chemicals and are available in extensive databases. Russel et al. [1], Pistikopoulos and Gani [2] described the interaction between different equations in a process model. In process simulation, the property models play a service role and are implemented as sub-models (as constitutive equations/phenomena models) into higher level process models as illustrated in figure 1. In general, measurable intensive variables (such as *T, P, x*) are calculated by the process models

and passed on as input to the phenomena models and constitutive equations. The phenomena models in turn compute the relevant thermodynamic and thermo-physical properties (e.g. γ, φ, P^{vap}), reaction rates or mass/energy transfer rates (stored in $\boldsymbol{\theta}$) as input to the process models.

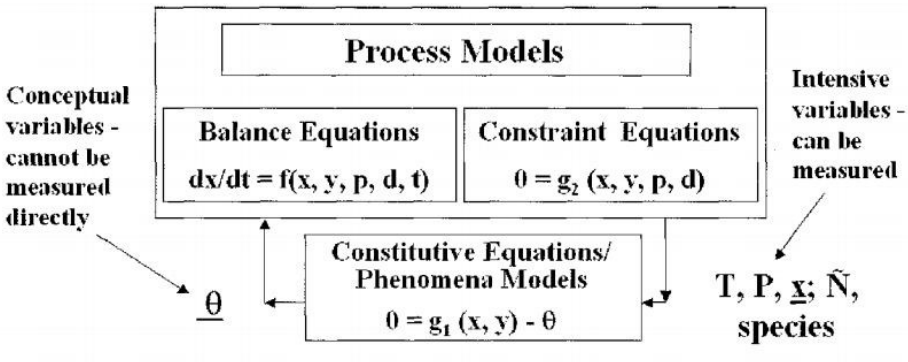

Figure 1: Classification of equations representing a process/product model and relationships between the different types of model equations [2]

Vector p accommodates all the (design) variables which are being calculated. d consists of all specified (design) variables making up the constraints/specifications related to the process. Variables in p and d are exchangeable although the degrees of freedom have to be satisfied and depends on which constraints have been set. It is self-evident that any inaccuracies or uncertainties in the phenomena model calculations will propagate and affect the process model calculations.

Dohrn and Pfohl [3] already discussed the importance of these aspects and outlined the industrial directions and future developments in regard to thermo-physical data provision and illustrate the problem of uncertainties in properties and how they lead to errors in the calculated design variables and thus affect investment costs. The importance of various properties depends on the unit operation put into perspective. This demands a pre-analysis of all properties which have a major influence on the operation and design while neglecting properties which don't have any impact. Since all properties are likely to have uncertainties associated with them, sensitivity analysis has to be performed to evaluate the effects of these uncertainties on design variables.

This sets the objective of this study and therefore a methodology is developed to verify if the property data in process design calculations are accurate enough or to recommend if further experiments have to be commissioned.

Sensitivity analysis can be described as 'the study of how the variation in the output of a mathematical model can be apportioned, qualitatively or quantitatively, to different sources of variation in the input of a model.' [4] Uncertainty originates from experimental errors and propagates over the parameter estimation of the model and numerous process design calculation steps. Although thermodynamic and thermo-physical models come along with a certain level of consistency and can be used over a certain range of conditions [5], the engineer has to be aware while designing a process that the choice of the correct model doesn't imply that the rigorous calculations will be free from uncertainty and the results can be taken for granted. The sensitivity analysis of process design is performed by taking the effect of uncertainties in estimated property values into account (which results due to uncertainties of the estimated model parameters of the property model).

As a sensitivity analysis the one-factor-at-a-time (OFAT) approach is used and the sensitivity of process design calculations to different properties are evaluated and ranked. From this

analysis it is possible to determine which properties are the most critical ones from process design point of view. The overall systematic methodology is applied to the process design of an extractive distillation column and the significance of the results are discussed and highlighted.

2. Systematic methodology for performing sensitivity analysis on process design due to uncertainties in property estimates

A systematic methodology is developed for performing analysis of sensitivity on process design due to uncertainties of the property estimates employed in the design calculations.
In the proposed method one property or design variable is perturbed while all other variables are kept fixed at their base case design values. This procedure is called the one-factor-at-a-time (OFAT) or local method for performing sensitivity analysis. The differential analysis can be described as follows:

$$S_{1,i,j}=\delta p/\delta \boldsymbol{\theta}_{i,j} \quad (1)$$

$$S_{2,k}=\delta p/\delta \underline{d}_k \quad (2)$$

After the differential analysis a ranking can be made for obtaining the most critical property and design variables. In addition, the chain rule is applied to obtain the sensitivity of a specified design variable to a property variable. An analytical connection is made because the needed relationship of design to property variables can not be realized with current process simulators:

$$S_{3,i,j,k}=S_{1,i,j,}*S_{2,k}^{-1}=\delta p/\delta \boldsymbol{\theta}_{i,j}*\delta \underline{d}_k/\delta p=\delta \underline{d}_k/\delta \boldsymbol{\theta}_{i,j} \quad (3)$$

This gives the user a pragmatic tool to predict how much a design variable may deviate due to uncertainties in property values. The process simulator Pro/II© 8.3 was used to perform sensitivity analysis on the base case design. As most simulators don't provide a sensitivity analysis tool for property variables, the perturbation of the property values has to be realized by calculating new parameters of the property correlations for the degree of perturbation wanted. The property value is perturbed to the desired value and a regression is performed to obtain the new parameters for the correlation. These new parameters are then entered into the process simulator to achieve the desired perturbation of a property.

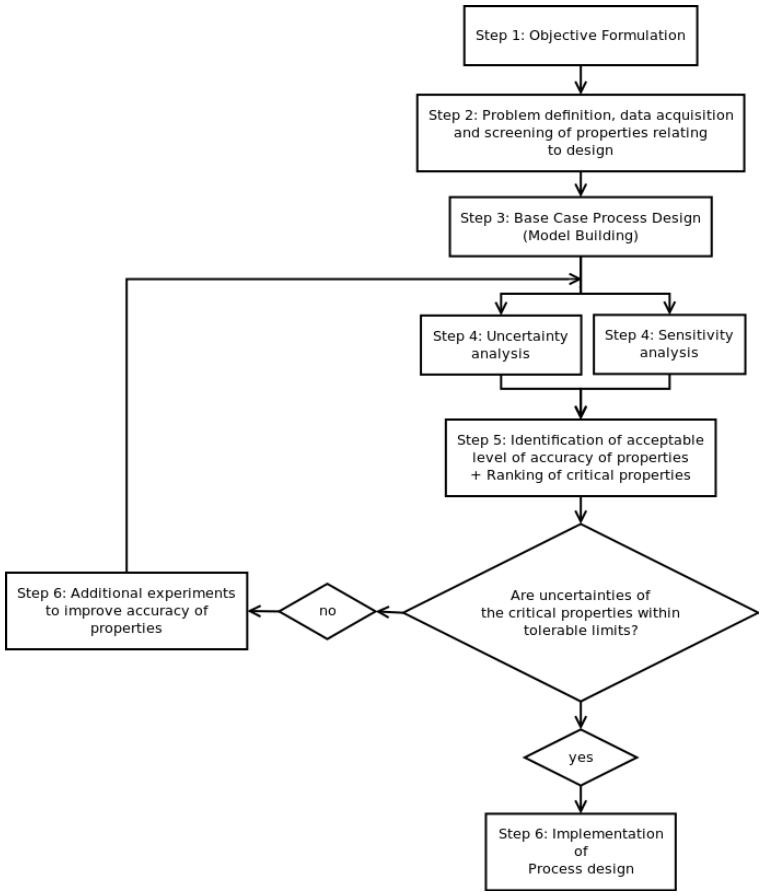

Figure 2: Systematic methodology for performing uncertainty and sensitivity analysis to evaluate acceptable uncertainties for critical properties

Figure 2 shows the developed methodology which consists of the following eight steps including the steps for sensitivity analysis:

Step 1: *Objective formulation*
The unit operation is specified and the desired process tasks (e.g. reaction, separation, heat-transfer) defined for which a sensitivity analysis has to be applied.

Step 2: *Problem description and data acquisition*
The chemical system involved is specified and the needed data for unit operation and process task (desired specifications, economical/environmental/operational constraints, kinetics, suitable thermo-physical and thermodynamic data) are collected.

Step 3: *Modeling, simulation and verification of the specified problem*
A modeling environment such as ICAS-MoT or a process simulator such as Pro/II© can be used to build a model for the specified problem. Process data (from literature or plant data) is taken for validation purposes. The process under study is modeled in terms of balance equations, constitutive equations and constraint equations. The model is solved numerically and the converged solution is verified for numerical accuracy.

Step 4: *Uncertainty analysis and sensitivity analysis*
Uncertainty and sensitivity analysis can be performed independently from each other and the results are being combined and interpreted in the next step. With uncertainty analysis the

uncertainty of each property is determined and with sensitivity analysis the most critical properties on the design are listed.

The sensitivity analysis can be divided into six steps (see Figure 3):

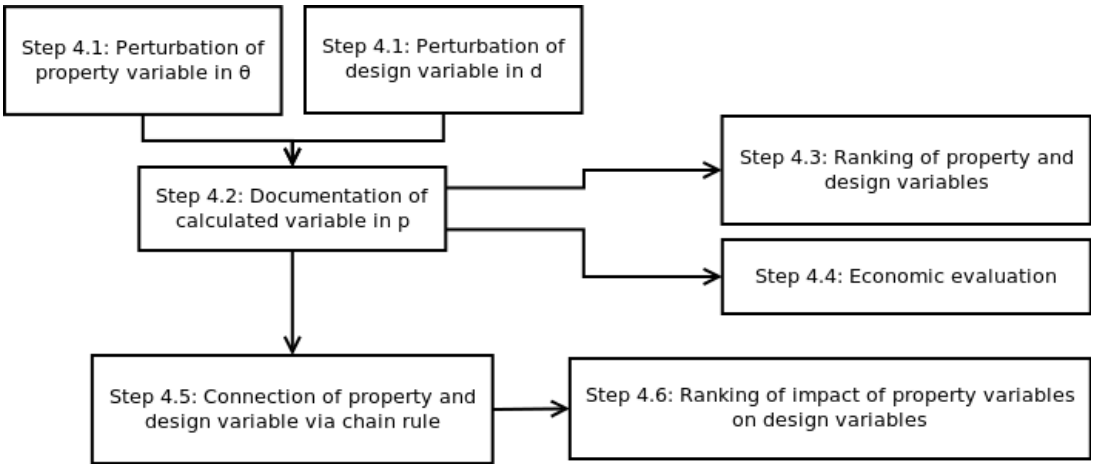

Figure 3: Sensitivity analysis

Step 4.1: *Perturbation of property and design variables*
The property variables stored in $\boldsymbol{\theta}$ or the design variables stored in $\underline{d}$ are perturbed. Only one variable either in $\boldsymbol{\theta}$ or $\underline{d}$ is perturbed at a time while all other variables in $\boldsymbol{\theta}$ and $\underline{d}$ are kept constant at their base case design value.

Step 4.2: *Documentation of calculated variable in p*
The calculated variable stored in p is documented for each perturbation of the previous step.

Step 4.3: *Ranking of property and design variables*
Sensitivity plots for $\delta p/\delta \boldsymbol{\theta}_{i,j}$ and $\delta p/\delta \underline{d}_k$ are obtained and the property and design variables can be ranked by their impact on the documented variable stored in p.

Step 4.4: *Economic evaluation*
An economic evaluation can be performed if the cost functions can be made dependent on the calculated variable in p.

Step 4.5: *Connection of property and design variable via chain rule*
The chain rule is applied to receive relationships between property variables and design variables:

$$S_{3,\,i,\,j,\,k}=S_{1,i,j,}*S_{2,k}^{-1}=\delta p/\delta \boldsymbol{\theta}_{i,j}*\delta \underline{d}_k/\delta p=\delta \underline{d}_k/\delta \boldsymbol{\theta}_{i,j} \qquad (4)$$

Step 4.6: *Ranking of relationships between property and design variables*
The most sensitive relationships between property and design variables are ranked.

Step 5: *Identification of acceptable uncertainty limits*
This step is the most crucial step of the methodology where the user defines the acceptable deviation for a design variable or for capital or operating cost. The acceptable uncertainty for important property values can then be defined based on the results of sensitivity analysis. If the uncertainty value of a specific property doesn't meet the user-defined requirements then additional experiments have to be performed to obtain more accurate property values and thus to reduce the uncertainty of the calculated design variables.

Step 6: *Additional experiments to improve accuracy of properties or implementation of design*
If the requirements were not met, uncertainty and sensitivity analysis have to be repeated after obtaining more accurate property values.
If all the uncertainties of all critical properties are within acceptable uncertainty limits then the process design can be implemented without the danger of infeasibility or poor performance due to uncertainties in the used property values.

The proposed methodology enables the user to identify the critical properties and determine if the uncertainty in the properties is acceptable or not. A refined schedule for experiments or a guideline for literature research can be set up for the properties which are defined as critical and don't meet the acceptable uncertainty limits.

3. Case study: extractive distillation

The methodology is applied to an extractive distillation process:

Step 1: *Objective formulation*
The objective in this case study is to determine the most sensitive property and design variables to uncertainties for an extractive distillation column and thus to perform a ranking. In addition an economic evaluation of uncertainties affecting capital cost (for column shell, a single tray and the condenser/reboiler) and the operating cost (for condenser/reboiler) has to be performed and relationships between property and design variables have to be evaluated.

Step 2: *Problem description and data acquisition*
The objective of the extractive distillation process is to produce 99 % pure acetone with a product flow rate of 76 kmol/hr.
The operating data is taken from Gil et al. [7] and summarized in the following table 1:

Table 1: Process data for base case design

Specifications	Values
Feed composition	$x_{Acetone}$=0.7775
	$x_{Methanol}$=0.2225
Feed temperature	293.15 K
Feed pressure	1 atm
Entrainer composition	x_{Water} = 1
Entrainer temperature	320.15 K
Entrainer pressure	1 atm
Loss of entrainer	0.4215 kmol/hr
Entrainer to feed ratio	2
Number of stages	52
Entrainer stage	22
Feed stage	48
Reflux ratio	5
Pressure drop per stage	0.01 atm
Thermodynamic property model	UNIQUAC

Table 2 summarizes all property variables of importance for distillation calculations, how they are obtained or calculated and for which calculations they are needed. The Pro/II© simulator uses the SIMSCI© property library to obtain single value pure component properties and temperature dependent properties.

Table 2: Summary of property variables for distillation design calculations

Property	Type	Calculated/Obtained by	Necessary for
Liquid activity coefficient γ	Thermodynamic	g^E-Model	K-Value (VLE)
Fugacity coefficient φ	Thermodynamic	EOS	K-Value (VLE)
Vapour pressure P^{vap}	Thermo-physical	Experiment/correlation/property estimation	K-Value (VLE)
Liquid and vapour enthalpy H^L, H^V	Thermo-physical	Experiment/correlation/property estimation	Energy balance
Heat of vapourization ΔH_V	Thermo-physical	Experiment/correlation/property estimation	Equipment sizing
Liquid density ρ	Thermo-physical	Experiment/correlation/property estimation	Equipment sizing
Viscosity μ	Thermo-physical	Experiment/correlation/property estimation	Equipment sizing
Surface tension σ	Thermo-physical	Experiment/correlation/property estimation	Equipment sizing
Critical temperature T_C	Fixed physical property	Experiment/property estimation	EOS/Thermo-physical Properties
Critical pressure P_C	Fixed physical property	Experiment/property estimation	EOS/Thermo-physical Properties
Acentric factor ω	Fixed physical property	Experiment/property estimation	EOS/Thermo-physical Properties

Step 3: *Modeling, simulation and verification of the specified problem*
A model of the base case was built in the process simulator Pro/II©, simulated and verified comparing the results of the case study from Gil et al.

Step 4: *Sensitivity analysis*

Step 4.1: *Perturbation of property and design variables*
Recoveries for the top and the bottom of the column are specified while reflux ratio and product flow rate are calculated. Performing the differential analysis on the base case design one property variable (e.g. P^{vap}, ΔH_V, ρ, μ and σ) is perturbed while all other variables are kept constant. The same procedure is followed for perturbing design variables (N_S, N_F *or* N_{oS}). The converged solutions of the performed perturbations have to satisfy the product purity and product flow rate constraints.

Step 4.2: *Documentation of calculated variable in p*
The calculated reflux ratio *RR* is then documented.
Figure 4 shows the results of the sensitivity analysis for the component vapour pressures. The vapour pressures of the high key (acetone) and low key (water) have the highest impact on the reflux ratio while the vapour pressure of the mid key (methanol) has little influence on the reflux ratio. It should be noted that the perturbation of the acetone vapour pressure rarely resulted in a converged solution. This demonstrates how sensitive the feasibility of a design is to uncertainties in the high key vapour pressure values.
Only two points for the perturbation of the acetone vapour pressure and five points for the perturbation of the water vapour pressure were obtained for the whole perturbation range (from -5% to +5% in steps of 0.5 %). In general, positive perturbations of the high key vapour pressure result in a decrease of the reflux ratio since the relative volatility between the high and low key increases ($\alpha > \alpha_0$). The opposite is the case for a decrease in the high key vapour pressure ($\alpha < \alpha_0$). Considering the low key, reflux ratio increases when perturbing the vapour pressure in the positive direction ($\alpha < \alpha_0$) and decreases for the negative side ($\alpha > \alpha_0$). The sensitivity plots in figure 4 illustrate the effect on the reflux ratio in absolute percentage. The x-axis is the deviation of the property variable from its base case design value in percentage. The y-axis is the effect of the perturbation (uncertainty) on the design variable. The plot on the left shows the effect on the reflux ratio by perturbing the acetone vapour pressure. A decrease of -0.25 % of the acetone vapour pressure from its base case design value leads to an increase in the reflux ratio of 48 %. A positive perturbation of the acetone vapour pressure by 1% causes the reflux ratio to decrease by 58 %. The plot on the right side shows the sensitivity of the reflux ratio to perturbations of the water vapour pressure. The perturbation of +0.75 % results in a 156 % increase in reflux ratio and a perturbation of -2 % decreases the reflux ratio by 64 %.

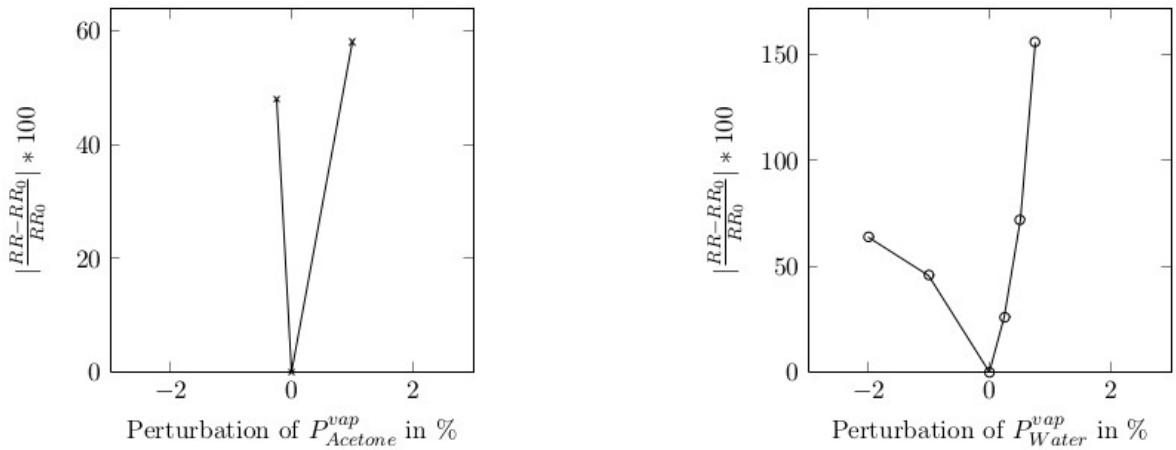

Figure 4: Perturbation of vapour pressure

Figure 5 indicates that perturbations of N_S and N_{oS} influence the reflux ratio RR. Simulations have shown that RR is insensitive to changes in N_F. Changes in the solvent feed stage increase the reflux ratio if the stage moves up the column thus decreasing the number of stages in the rectifying section. Increasing the number of stages in the rectifying section by moving the solvent entry stage downwards decreases the reflux ratio. In comparison to the changes in N_S the perturbation of N_{oS} shows the same form of sensitivity for the reflux ratio.

Step 4.3: *Ranking of property and design variables*
A ranking of the most sensitive property and design variables can be performed and table 3 shows that for negative uncertainties the reflux ratio is most sensitive to uncertainties in the vapour pressure of acetone followed by the vapour pressure in water. For positive uncertainties the vapour pressure of water has the highest impact on reflux ratio followed by the vapour pressure of acetone. The solvent stage position is the design variable to which reflux ratio is most sensitive both for negative and positive uncertainties followed by the number of stages.

Table 3: Ranking of property and design variables

Negative uncertainty	Effect on reflux ratio (RR)	Positive uncertainty	Effect on reflux ratio (RR)
-0.25 % in $P^{vap}_{Acetone}$	48.0 %	+0.75 % in P^{vap}_{Water}	156.0 %
-1.0 % in P^{vap}_{Water}	46.0 %	+1.0 % in $P^{vap}_{Acetone}$	58.0 %
-27.3 % in N_S	94.0 %	+22.7 % in N_S	18.0 %
-28.8 % in N_{oS}	86.0 %	+23.1 % in N_{oS}	18.0 %

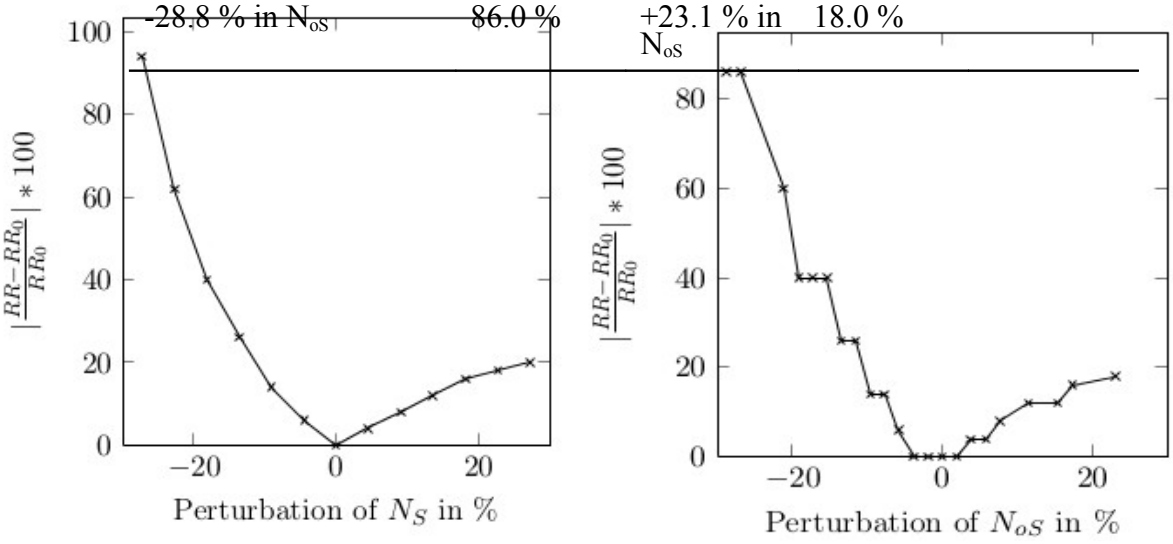

Figure 5: Perturbation of solvent stage position and number of stages

Step 4.4: *Economic evaluation*

The relatively small changes in vapour pressure have a large impact on the reflux ratio and thus on the equipment and operating cost of the column as can be seen in the plots of figure 6. The left plot shows that a deviation of -0.25% for the acetone vapour pressure results in an increase by 18-41% in equipment cost and 40% in operating cost. A deviation of 1 % in the positive direction results in a decrease by 11-27 % in equipment cost and 40% decrease in operating cost.

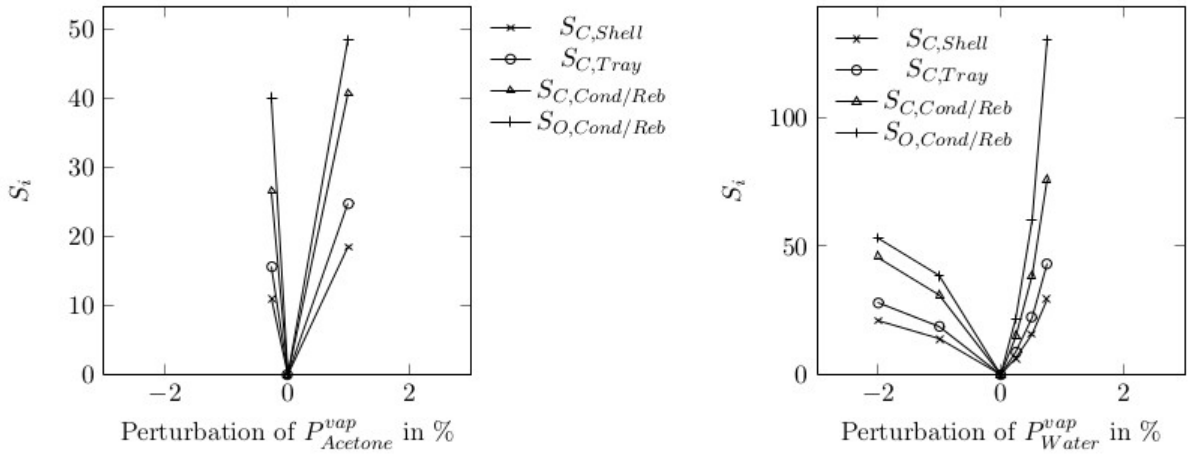

Figure 6: Economic evaluation of perturbations of vapour pressures

For the design variables it can be noted that the operating cost is most sensitive to perturbations of the solvent stage followed by the equipment cost (capital cost) for the condenser and reboiler, the capital cost for the trays and last the capital cost for the column shell. In comparison to changes in N_S the perturbation of N_{oS} shows the same form of sensitivity for the reflux ratio (figure 5). However the reflux ratio is less sensitive to N_{oS} than to N_S and thus $S_{C,Shell}$, $S_{C,Tray}$, $S_{C,Cond/Reb}$ and $S_{O,Cond/Reb}$ are less sensitive to changes in N_{oS} (figure 7). For the negative perturbation of N_{oS} the sensitivity plot of $C_{C,Shell}$ (figure 8) shows fluctuations since RR and N_{oS} are used in the cost calculation for the shell (see Appendix).

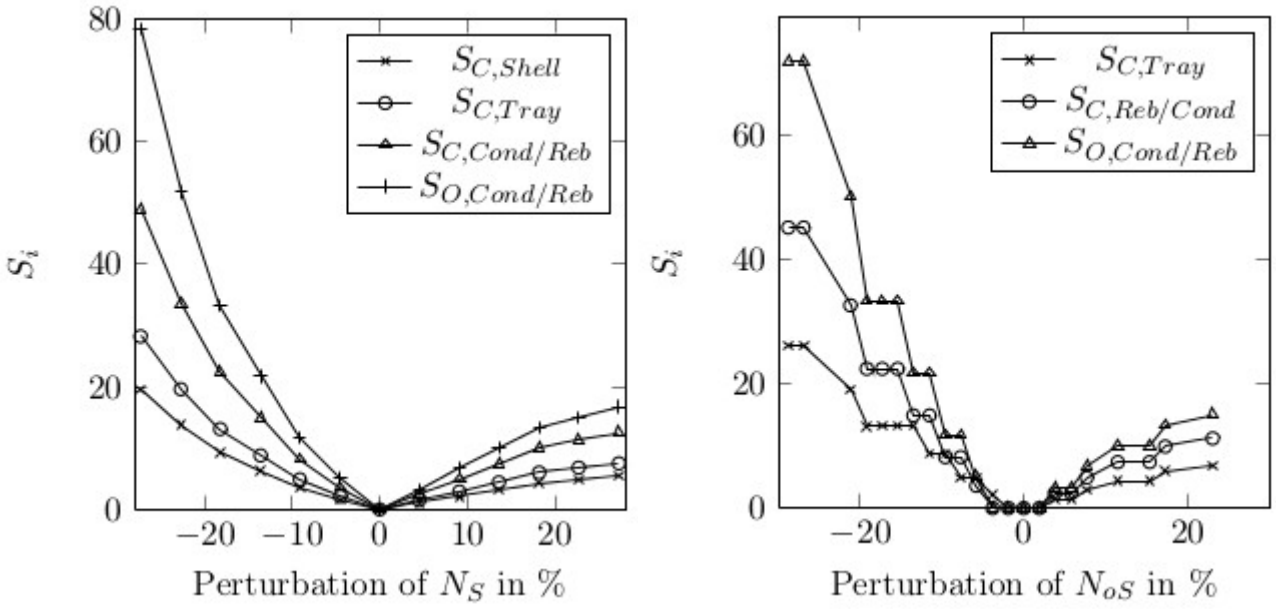

Figure 7: Economic evaluation of perturbations of solvent stage position and number of stages

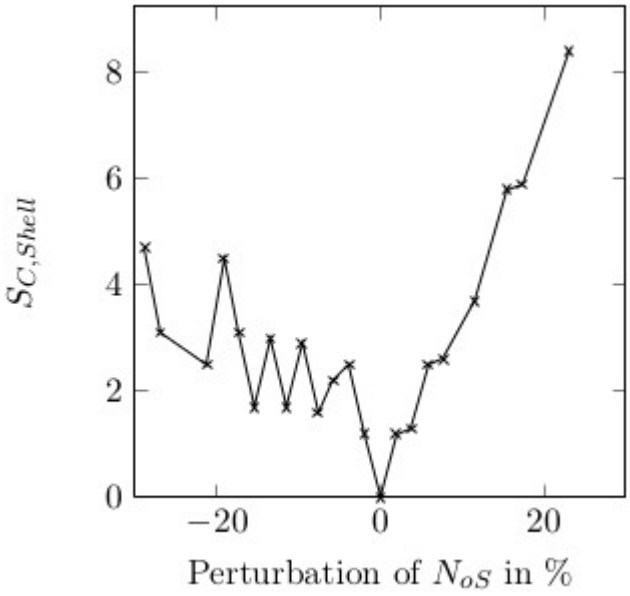

Figure 8: Effect of perturbations of number of stages on the capital cost of the column shell

Step 4.5: *Connection of property and design variable*
By connecting the specified design variables with the properties variables via the chain rule it is possible to obtain relationships which can't currently be obtained by process simulators. Table 4 shows the sensitivity of the design variables N_S or N_{oS} to the property variable P^{vap}_i. The procedure of obtaining the deviations can be described analytically as follows:

$$\Delta RR/\Delta P^{vap}_i * (\Delta RR/\Delta N_S)^{-1} = \Delta N_S/\Delta P^{vap}_i \quad (4)$$
$$\Delta RR/\Delta P^{vap}_i * (\Delta RR/\Delta N_{oS})^{-1} = \Delta N_{oS}/\Delta P^{vap}_i \quad (5)$$

It is important to note that ΔRR is of the same value and the same sign for both sensitivity terms in the above equations. Perturbing the high key vapour pressure in negative direction is

equivalent to a decrease in the solvent feed stage position or a decrease in the number of stages. The results show that if the vapour pressure value of acetone has an uncertainty of -0.25% then the solvent stage position can deviate about 18.2 % and the number of stages can deviate up to 19.2% from the base case design.

Table 4: Sensitivity of design variables to component vapour pressures

Property variable	P^{vap}_i			
Perturbation of property variable	-0.25 %	0 %	+0.25 %	+0.5 %
ΔN_S [%] for Acetone	18.2	0	-	-
ΔN_S [%] for Water	-	0	13.6	27.3
ΔN_{oS} [%] for Acetone	19.2	0	-	-
ΔN_{oS} [%] for Water	-	0	11.5-13.5	21.2

The perturbation of the low key vapour pressure in positive direction equals a decrease in the solvent feed stage position or a decrease in the number of stages. Uncertainty in the vapour pressure value of water from +0.25% to +0.5% can imply a deviation in the solvent feed stage position of 13.6% to 27.3% and number of stages from 11.5% to 21.2 %.

Step 4.6: *Ranking of relationships between property and design variables*
A ranking is performed by using the results of the previous step. Table 5 ranks the relationships from top to bottom and illustrates that a negative perturbation of -0.25 % of the acetone vapour pressure corresponds to a decrease of 19.2 % in number of stages. The same perturbation corresponds to a decrease of the rectifying section by moving the solvent stage position 18.2 % upwards. The positive perturbation of 0.5 % of the water vapour pressure complies a decrease of the rectifying section by moving the solvent stage position 27.3 % upwards from its original position followed by the less sensitive number of stages complying with a decrease of 21.2 %.

Table 5: Ranking of relationships between property and design variables

Negative perturbation of	Effect on	Positive perturbation of	Effect on
-0.25 % of $P^{vap}_{Acetone}$	ΔN_{oS} by 19.2 %	+0.5 % of P^{vap}_{Water}	ΔN_S by 27.3 %
-0.25 % of $P^{vap}_{Acetone}$	ΔN_S by 18.2 %	+0.5 % of P^{vap}_{Water}	ΔN_{oS} by 21.2 %

Step 5: *Identification of acceptable uncertainty limits*
The user can define acceptable deviations of the reflux ratio or costs and determine how high the allowed uncertainty in vapour pressure can be. Figure 9 illustrates this procedure.

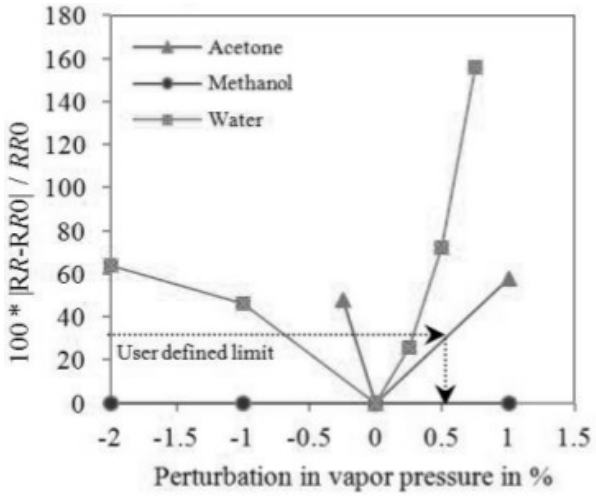

Figure 9: Identification of user defined uncertainty limits [8]

Step 6: *Additional experiments to improve accuracy of properties or implementation of design*

By comparing the uncertainty limits with the uncertainties in the property variables the user can state if additional experiments have to be performed for obtaining more accurate property values or the design is accepted with the current level of uncertainty in the performance metrics. An improved reliability of the design is in principle possible if the uncertainties in property data can be brought below the defined uncertainty limits.

4. Conclusion

A systematic methodology for analyzing the effects of uncertainties in property estimates on process design has been developed and applied to a case study of an extractive distillation column. Uncertainty and sensitivity analysis can be combined to determine the most important variables and their acceptable uncertainties. A model to evaluate the sensitivity of capital and operating cost to uncertainties in physical properties has also been proposed. Finally, the application of the proposed methodology illustrates that uncertainties in physical property values can have significant impact on the design and economics of an extractive distillation column. Chemical as well as biochemical process design calculations will immensely benefit from systematic treatment of uncertainties for better informed and reliable generation of design solutions.

Nomenclature
P pressure
R universal gas constant
T temperature
EOS equation of state
g^E Gibbs free energy
x molar liquid composition
γ liquid activity coefficient

φ fugacity coefficient

P^{vap} vapour pressure

$\boldsymbol{\Theta}$ matrix of property variables

p calculated (design) variable

$\underline{d}$ vector of specified (design) variables

$\underline{x}$ vector of intensive variables (process variables)

$\underline{y}$ vector of measureable variables (process variables)

H^L liquid enthalpy

H^V vapour enthalpy

ΔH_V heat of vapourization

ρ density

μ liquid viscosity

σ surface tension

T_C critical temperature

P_C critical pressure

ω acentric factor

N_S number of solvent stage

N_F number of feed stage

N_{oS} number of stages

RR reflux ratio

D sizing variable

A_{Cond} condenser heat transfer area

A_{Reb} reboiler heat transfer area

C_i cost of equipment piece

$C_{Cooling\ Water}$ cost of cooling water

ε_i exponent for equipment cost vs. capacity

$C_{0,i}$ cost of equipment piece from base case design

$C_{C,i}$ capital cost of equipment piece

$\rho_{Material}$ density of material

H_{TS} tray stack height

Δw thickness of shell

d column diameter

$Cost_{Material}$ cost for material used for the column shell

A_{Tray}	column shell tray area
F_V	vapour flow rate at the top of the column
v_m	vapour velocity
F_P	product flow rate
N_{oS}	number of stages
N_S	number of solvent stage
N_F	number of feed stage
Q_{Cond}	heat duty of condenser
U_{HX}	heat transfer coefficient
ΔT_m	temperature difference between hot and cold stream
κ	correlation factor

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Appendix Economic evaluation

In respect of sensitivity analysis the relative change of the reflux ratio to the nominal reflux ratio is of interest. The same is valid for the economic evaluation where the sensitivities of the costs to changes in thermo-physical and thermodynamic properties are determined by using the reflux ratio as the connecting variable. In the case of the extractive distillation column four key sizing variables (D) have to be specified to obtain the overall cost of the column. These are the column diameter d, the column height h, the condenser area A_{Cond} and the reboiler area A_{Reb}. All four sizing variables can be expressed as a function of the reflux ratio. When designing a distillation column the optimal reflux ratio is obtained by minimizing total cost. The total annual cost for the extractive distillation column is made up of the capital and operating cost. The capital cost includes the column shell and tray costs and the cost for the heat exchangers for reboiling and condensing. The operating cost consists of the cost of cooling water for the condenser and the cost of steam for the reboiler. To obtain relative investment cost changes from a base case to a modified design, typical scaling equations are widely used in the chemical industry [9]:

$$C/C_0 = (D/D_0)^{\varepsilon}$$

The capital cost for the column shell $C_{C,Shell}$ and trays $C_{C,Tray}$ can be expressed with the following expressions [10]:

$$C_{C,Shell} = \rho_{Material} * H_{TS} * \Delta w * \pi * d/2 * Cost_{Material}$$

$$C_{C,Tray} = d * Cost_{Tray}$$

Where H_{TS} is defined as the tray stack height including tray spacing, extra feed space, disengagement space and skirt height [10]:

$$H_{TS} = (N_{oS}\text{-}1) * \text{Tray Spacing} + \text{Extra Feed Space} + \text{Disengagement Space} + \text{Skirt Height}$$

Thus, a relative term for the capital cost of the column shell can be stated as:

$$C_{C,Shell}/C_{0,C,Shell} = ((\rho_{Material} * H_{TS} * \Delta w * \pi * d/2 * Cost_{Material})/(\rho_{Material} * H_{0,TS} * \Delta w * \pi * d_0/2 * Cost_{Material}))^{\varepsilon,Shell}$$

Since only the diameter or the number of stages changes with perturbation of an affecting property value the term simplifies to:

$$C_{C,Shell}/C_{0,C,Shell} = (((N_{oS} - 1) * d)/((N_{0,oS} - 1) * d_0))^{\varepsilon,Shell}$$

The tray diameter can be expressed as a function of reflux ratio [11]:

$$A_{Tray} = F_V/v_m = \pi * (d/2)^2$$

$$d = 2 * sqrt(F_V/(v_m * \pi))$$

Where F_V is the maximal volumetric vapour flow rate assumed being at the top of the column and can be expressed in terms of RR as follows:

$$F_V = F_P * RR + F_P = F_P * (RR + 1)$$

and thus:

$$d = 2*sqrt((F_P*(RR+1))/(v_m*\pi))$$

Finally, the relative capital cost change for the column shell can be expressed as:

$$C_{C,Shell}/C_{0,C,Shell} = ((N_{oS}-1)*d/(N_{0,oS}-1)*d_0)^{\varepsilon,Shell} = (((N_{oS}-1)*(RR+1))/((N_{0,oS}-1)*(RR_0+1)))^{\varepsilon,Shell}$$

Since the deviation from the base case design is often desired in a percentage for sensitivity analysis the term needs to be modified to:

$$S_{C,Shell} = (C_{C,Shell} - C_{0,C,Shell}) / C_{0,C,Shell} * 100 = ((RR-RR_0)/(RR_0+1))^{\varepsilon,Shell}*100$$

The same procedure can be applied to the sensitivity of the tray cost and the following expression is obtained:

$$S_{C,Tray} = (C_{C,Tray} - C_{0,C,Tray})/C_{0,C,Tray} *100 = ((RR-RR_0)/(RR_0 + 1))^{\varepsilon,Shell}*100$$

The capital cost of the condenser and reboiler depends on the heat exchanger areas which can be calculated from the following relationship [10]:

$$Q_{Cond} = U_{HX}*A_{Cond}*\Delta T_m$$
$$A = Q/(U_{HX}*\Delta T_m) = (F_V*\Delta H_V)/(U_{HX}*\Delta T_m)$$

$$Q_{Reb} = \kappa*Q_{Cond}$$

where κ is a correlation factor between the condenser and the reboiler heat duty. In relative terms the relationships are stated as:

$$C_{C,Cond}/C_{0,C,Cond} = (A_{Cond}/A_{0,Cond})^{\varepsilon,Heat\ Exchanger} = (V/V_0)^{\varepsilon,Heat\ Exchanger}$$
$$= ((RR*(F_P+1)/(RR_0*(F_P+1)))^{\varepsilon,Heat\ Exchanger} = (RR/RR_0)^{\varepsilon,Heat\ Exchanger}$$

$$C_{C,Reb}/C_{0,C,Reb} = C_{C,Cond}/C_{0,C,Cond} = ((RR*(F_P+1))/RR_0*(F_P+1))^{\varepsilon,Heat\ Exchanger} = (RR/RR_0)^{\varepsilon,Heat\ Exchanger}$$

For sensitivity analysis the equations have to be modified to:

$$S_{C,Cond/Reb} = (C_{C,Cond/Reb} - C_{0,C,Cond/Reb})/C_{0,C,Cond//Reb} = ((RR-RR_0)/RR_0)^{\varepsilon,Heat\ Exchanger}*100$$
$$= (RR/RR_0 - 1)^{\varepsilon,Heat\ Exchanger}*100$$

Thus, changes in reflux ratio have the same relative effect on the condenser and reboiler heat duties and on the condenser and reboiler heat transfer areas. The operating cost consists of the costs for the cooling water for condensing and the steam for reboiling which are given by the following equations [11]:

$$C_{O,Cond} = C_{Cooling\ Water} * F_V = C_{Cooling\ Water} * F_P*(RR+1)$$

$$C_{O,Reb} = \kappa * C_{O,Cond}$$

and thus in relative terms the equations are:

$$C_{O,Cond}/C_{0,O,Cond} = (F_P*(RR+1))/(F_P*(RR_0+1)) = (RR+1)/(RR_0+1)$$

$C_{O,Reb}/C_{0,O,Reb} = C_{O,Cond} / C_{0,O,Cond} = (RR + 1)/(RR_0 + 1)$

For sensitivity analysis the previous equations are modified to:

$S_{O,Cond/Reb} = (C_{O,Cond/Reb} - C_{0,O,Cond/Reb})/C_{0,O,Cond/Reb} * 100 = (RR - RR_0)/(RR_0 + 1) * 100$

The specific exponents for equipment cost calculations are [9]:

$\varepsilon_{Shell} = 0.62$

$\varepsilon_{Sieve\ Tray} = 0.86$

$\varepsilon_{Heat\ Exchanger} = 0.6$